PHY 770 -- Statistical Mechanics
12:00-1:45 PM TR Olin 107

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Lecture 12 -- Chapter 5
Equilibrium Statistical Mechanics
Canonical ensemble

- Magnetic effects
- Ising model

3	Tue: 01/21/2014	Chap. 3	Thermodynamic potentials	#3	02/04/2014
4	Tue: 01/21/2014	Chap. 3	Thermodynamic stability	#4	02/04/2014
5	Thu: 01/23/2014	Chap. 3	Thermodynamic stability	#5	02/04/2014
	Tue: 01/28/2014		NAWH out of town - no class		
	Thu: 01/30/2014		NAWH out of town - no class		
6	Tue: 02/04/2014	Chap. 4	Phase transitions	#6	02/11/2014
7	Thur: 02/06/2014	Chap. 2	Microscopic analysis of entropy	#7	02/11/2014
8	Thur: 02/06/2014	Chap. 2	Microscopic analysis of entropy	#8	02/11/2014
9	Tue: 02/11/2014	Chap. 2	Microscopic analysis of entropy	#9	02/18/2014
	Thur: 02/13/2014		Class cancelled due to weather		
10	Tue: 02/18/2014	Chap. 5	Equilibrium Statistical Mechanics	#10	02/27/2014
11	Tue: 02/18/2014	Chap. 5	Equilibrium Statistical Mechanics	#11	02/27/2014
12	Thur: 02/20/2014	Chap. 5	The Ising model (class 12-1:45 PM)	#12	02/27/2014
	Tue: 02/25/2014		NAWH out of town -- no class		
13	Thur: 02/27/2014	Chap. 5	(class 12-1:45 PM)		
	Tue: 03/04/2014	*APS Meeting*	Take-home exam (no class meeting)		
	Thur: 03/06/2014	*APS Meeting*	Take-home exam (no class meeting)		
	Tue: 03/11/2014		Spring break (no class meeting)		
	Thur: 03/13/2014		Spring break (no class meeting)		
14	Tue: 03/18/2014	Chap. 6	(Exam due)		

Summary of results for the canonical ensemble

$$\hat{\rho} = \frac{\exp\left(-\frac{\hat{H}}{k_B T}\right)}{Z(T)} \quad \text{where } Z(T) = \mathrm{Tr}\left[\exp\left(-\frac{\hat{H}}{k_B T}\right)\right]$$

$$A = -k_B T \ln\left(Z(T)\right) \quad \Rightarrow \hat{\rho} = \exp\left(-\frac{\hat{H}-A}{k_B T}\right) \equiv \exp\left(-\beta(\hat{H}-A)\right)$$

$$S = -k_B \,\mathrm{Tr}\left[\hat{\rho}\ln\left(\hat{\rho}\right)\right]$$

$$U = \mathrm{Tr}\left[\hat{\rho}\hat{H}\right]$$

Canonical ensemble – example including magnetic effects

Consider a system of N particles in a box of volume V, treated in the semiclassical limit. Since we are in the semiclassical limit, we can use the relationship

$$Z_N(T)=\frac{1}{N!}\left(Z_1(T)\right)^N$$

$$\text{where } Z_1(T)=\text{Tr}\left[\exp\left(-\frac{\hat{H}_1}{k_BT}\right)\right]\equiv\text{Tr}\left[\exp\left(-\beta\hat{H}_1\right)\right]$$

$$\hat{H}_1=\frac{\mathbf{p}^2}{2m}+\mu sB\equiv\hat{H}_{1(trans)}+\hat{H}_{1(\text{mag})}$$

here, B denotes the magnetic field strength

μ denotes the magnetic moment factor

$s=\pm\frac{1}{2}$ denotes the intrinsic spin

Canonical ensemble – example including magnetic effects -- continued

$$Z_1(T)=\text{Tr}\left[\exp\left(-\beta\left(\hat{H}_{1(trans)}+\hat{H}_{1(\text{mag})}\right)\right)\right]=Z_{1(trans)}(T)Z_{1(mag)}(T)$$

$$Z_{1(trans)}(T)=\left(\frac{V}{\lambda_T^3}\right)$$

$$Z_{1(mag)}(T)=e^{-\beta\mu B/2}+e^{\beta\mu B/2}=2\cosh\left(\beta\mu B/2\right)$$

$$Z_N(T)=\frac{1}{N!}\left(\frac{2V}{\lambda_T^3}\right)^N\cosh^N\left(\beta\mu B/2\right)$$

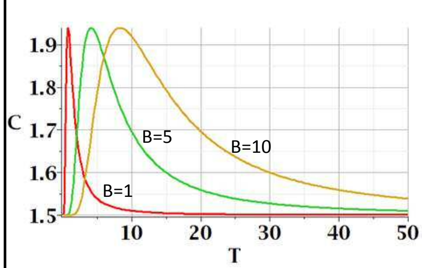
$$U=-\left(\frac{\partial\ln\left(Z_N(T)\right)}{\partial\beta}\right)=\frac{3}{2}Nk_BT-\frac{1}{2}N\mu B\tanh\left(\beta\mu B/2\right)$$

$$C_{V,N,B}=\left(\frac{\partial U}{\partial T}\right)_{V,N,B}=\frac{3}{2}Nk_B+Nk_B\left(\frac{\beta\mu B}{2}\right)^2\text{sech}^2\left(\frac{\beta\mu B}{2}\right)$$

$$\text{Magnetization:}\quad M=\left(\frac{\partial\left(k_BT\ln\left(Z_N(T)\right)\right)}{\partial B}\right)_{T,V,N}=\frac{N\mu}{2}\tanh\left(\frac{\beta\mu B}{2}\right)$$

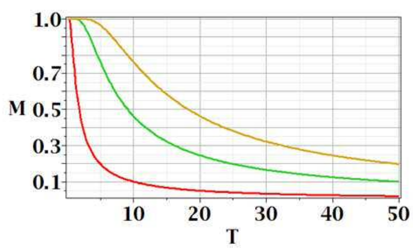
Canonical ensemble – example including magnetic effects -- continued

$$C_{V,N,B}=\frac{3}{2}Nk_B+Nk_B\left(\frac{\beta\mu B}{2}\right)^2\text{sech}^2\left(\frac{\beta\mu B}{2}\right)$$



Canonical ensemble – example including magnetic effects -- continued

$$M = \left(\frac{\partial \left(k_B T \ln \left(Z_N (T) \right) \right)}{\partial B} \right)_{T,V,N} = \frac{N\mu}{2} \tanh\left(\frac{\beta \mu B}{2} \right)$$



Statistical mechanics of the Ising model

Spin ½ system with competing effects of nearest-neighbor interactions and spin alignment energy in a magnetic field

Spin alignment contribution (convenient redefinition of "s")

$$\hat{H}_B = -\mu \left(\sum_i s_i \right) B \quad \text{where } s_i = \pm 1, \;\; \mu B \equiv \text{ spin alignment energy}$$

$$\mu \equiv \tfrac{1}{2} g \mu_B = -9.28 \times 10^{-24} J/T \quad \text{(for an electron)}$$

Partition function for $\hat{H}_B$ term alone for N non-interacting spins:

$$Z_N = \sum_{s_1=\pm1} \sum_{s_2=\pm1} \sum_{s_3=\pm1} \cdots \sum_{s_N=\pm1} e^{\beta \mu B \left(\sum_{i=1}^{N} s_i \right)}$$

$$= \left(\sum_{s_1=\pm1} e^{\beta \mu B s_1} \right)^N = \left(Z_1 \right)^N$$

Calculation of Z_1

$$Z_1 = \sum_{s_1=\pm1} e^{\beta \mu B s_1} = e^{-\beta \mu B} + e^{\beta \mu B} = 2\cosh(\beta \mu B)$$

Thermodynamic functions:

$$A = -kT \ln\left(Z_1 \right)^N = -NkT \ln Z_1 = -NkT \ln\left(2\cosh(\beta \mu B) \right)$$

$$U = -N \frac{\partial \ln Z_1}{\partial \beta} = -N \mu B \tanh\left(\beta \mu B \right)$$

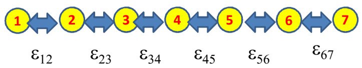
$$C = \left(\frac{\partial U}{\partial T} \right)_B = kN \left(\beta \mu B \right)^2 \operatorname{sech}^2 \left(\beta \mu B \right)$$

Statistical mechanics of the Ising model -- continued

Spin ½ system with competing effects of nearest-neighbor interactions and spin alignment energy in a magnetic field

Nearest-neighbor interaction term:

$$\hat{H}_{int} = \sum_{i,j(nn)}^{N} \epsilon_{ij} s_i s_j$$



Ising model:

$$\hat{H}_{Ising} = \hat{H}_{int} + \hat{H}_B = \sum_{i,j(nn)}^{N} \epsilon_{ij} s_i s_j - \mu B \sum_{i=1}^{N} s_i$$

Ising model – effects of interaction term alone for N=2; $\varepsilon_{ij}=\varepsilon$

$$\hat{H}_{int} = -\epsilon \sum_{i,j(nn)}^{N} s_i s_j$$

$$\left\langle \hat{H}_{int} \right\rangle = \quad -\epsilon \quad -\epsilon \quad +\epsilon \quad +\epsilon$$

$$Z_2 = e^{\beta\varepsilon} + e^{\beta\varepsilon} + e^{-\beta\varepsilon} + e^{-\beta\varepsilon} = 4\cosh(\beta\varepsilon)$$

$$U = -\frac{\partial \ln Z_2}{\partial \beta} = -\varepsilon \tanh(\beta\varepsilon)$$

Ising model -- full model for N=2; $\varepsilon_{ij}=\varepsilon$

$$\hat{H}_{\text{Ising}} = -\epsilon \sum_{i,j(nn)}^{2} s_i s_j - \mu B \sum_{i=1}^{2} s_i$$

$$\left\langle \hat{H}_{int} \right\rangle = \quad -\epsilon \quad -\epsilon \quad +\epsilon \quad +\epsilon$$

$$Z_2(\varepsilon, B) = e^{\beta(\varepsilon + 2\mu B)} + e^{\beta(\varepsilon - 2\mu B)} + e^{-\beta\varepsilon} + e^{-\beta\varepsilon}$$
$$= 2e^{\beta\varepsilon}\cosh(2\beta\mu B) + 2e^{-\beta\varepsilon}$$

Partition function for 1-dimensional Ising system of *N* spins with periodic boundary conditions ($s_{N+1}=s_1$)

$$Z_N = \mathrm{Tr}\left[\exp\left(\beta\varepsilon\sum_{i=1}^{N} s_i s_{i+1} + \frac{\beta\mu B}{2}\sum_{i=1}^{N}\left(s_i + s_{i+1}\right)\right)\right]$$

$$\equiv \sum_{s_1, s_2, s_3 \cdots s_N} f(s_1, s_2) f(s_2, s_3) \cdots f(s_{N-1}, s_N) f(s_N, s_{N+1})$$

where:

$$f(s, s') = \begin{pmatrix} f(1,1) & f(1,-1) \\ f(-1,1) & f(-1,-1) \end{pmatrix}$$

$$\equiv \begin{pmatrix} e^{(\beta\varepsilon+\beta\mu B)} & e^{(-\beta\varepsilon)} \\ e^{(-\beta\varepsilon)} & e^{(\beta\varepsilon-\beta\mu B)} \end{pmatrix} \equiv \overline{\mathbf{P}}$$

1-dimensional Ising system of *N* spins with periodic boundary conditions ($s_{N+1}=s_1$) (continued)

$$Z_N = \sum_{s_1, s_2, s_3 \cdots s_N} f(s_1, s_2) f(s_2, s_3) \cdots f(s_{N-1}, s_N) f(s_N, s_{N+1})$$

$$= \sum_{s_1, s_2, s_3 \cdots s_N} \overline{P}_{s_1 s_2} \overline{P}_{s_2 s_3} \overline{P}_{s_3 s_4} \overline{P}_{s_4 s_5} \cdots \overline{P}_{s_N s_{N+1}}$$

where:

$$\overline{\mathbf{P}} \equiv \begin{pmatrix} e^{(\beta\varepsilon+\beta\mu B)} & e^{(-\beta\varepsilon)} \\ e^{(-\beta\varepsilon)} & e^{(\beta\varepsilon-\beta\mu B)} \end{pmatrix}$$

$$Z_N = \mathrm{Tr}\left[\overline{\mathbf{P}}^N\right]$$

1-dimensional Ising system of *N* spins with periodic boundary conditions ($s_{N+1}=s_1$) (continued)

Some tricks from linear algebra:

1. Any symmetric matrix $\mathbf{T}$ can be diagonalized by a transformation of the type $\mathbf{U}^{-1}\mathbf{T}\mathbf{U} = \mathbf{\Lambda} \equiv \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \lambda_n \end{pmatrix}$.
2. $\mathbf{TTT}\cdots\mathbf{T} = \mathbf{TUU}^{-1}\mathbf{TUU}^{-1}\mathbf{TU}\cdots\mathbf{U}^{-1}\mathbf{T}$
3. $\mathrm{Tr}(\mathbf{TTT}\cdots\mathbf{T}) = \mathrm{Tr}(\mathbf{U}^{-1}\mathbf{TTT}\cdots\mathbf{TU}) = \mathrm{Tr}(\mathbf{\Lambda\Lambda}\cdots\mathbf{\Lambda})$

$$\Rightarrow \mathrm{Tr}\left[\overline{\mathbf{P}}^N\right] = \lambda_1^N + \lambda_2^N$$

1-dimensional Ising system of N spins with periodic boundary conditions ($s_{N+1}=s_1$) (continued)

In this case:

$$\bar{\mathbf{P}} \equiv \begin{pmatrix} e^{(\beta\varepsilon+\beta\mu B)} & e^{(-\beta\varepsilon)} \\ e^{(-\beta\varepsilon)} & e^{(\beta\varepsilon-\beta\mu B)} \end{pmatrix}$$

$$\boldsymbol{\Lambda} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

$$\lambda_1 = e^{\beta\varepsilon}\left\{\cosh(\beta\mu B) + \left[\sinh^2(\beta\mu B) + e^{-4\beta\varepsilon}\right]^{1/2}\right\}$$

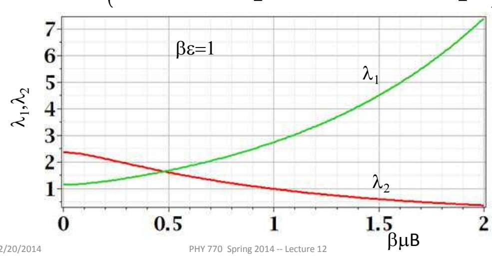
$$\lambda_2 = e^{\beta\varepsilon}\left\{\cosh(\beta\mu B) - \left[\sinh^2(\beta\mu B) + e^{-4\beta\varepsilon}\right]^{1/2}\right\}$$

$$Z_N = \mathrm{Tr}\left(\bar{\mathbf{P}}^N\right) = \lambda_1^N + \lambda_2^N$$

1-dimensional Ising system of N spins with periodic boundary conditions ($s_{N+1}=s_1$) (continued)

$$\lambda_1 = e^{\beta\varepsilon}\left\{\cosh(\beta\mu B) + \left[\sinh^2(\beta\mu B) + e^{-4\beta\varepsilon}\right]^{1/2}\right\}$$

$$\lambda_2 = e^{\beta\varepsilon}\left\{\cosh(\beta\mu B) - \left[\sinh^2(\beta\mu B) + e^{-4\beta\varepsilon}\right]^{1/2}\right\}$$



1-dimensional Ising system of N spins with periodic boundary conditions ($s_{N+1}=s_1$) (continued)

$$Z_N = \mathrm{Tr}\left(\bar{\mathbf{P}}^N\right) = \lambda_1^N + \lambda_2^N = \lambda_1^N\left(1 + \left(\frac{\lambda_2}{\lambda_1}\right)^N\right)$$

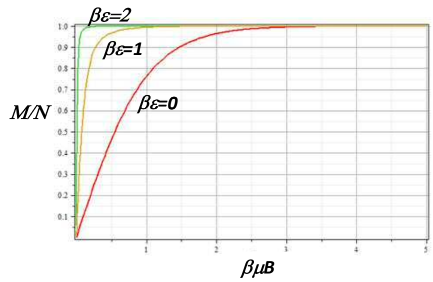
$$A(T,\varepsilon,B) = -kT\ln Z_N = -NkT\ln\lambda_1 - kT\ln\left[1 + \left(\frac{\lambda_2}{\lambda_1}\right)^N\right]$$

$$\approx -NkT\ln\lambda_1$$

$$= -N\varepsilon - kT\ln\left[\cosh(\beta\mu B) + \left[\sinh^2(\beta\mu B) + e^{-4\beta\varepsilon}\right]^{1/2}\right]$$

$$M(T,\varepsilon,B) = -\frac{\partial A}{\partial B} = \frac{N\mu\sinh(\beta\mu B)}{\left[\sinh^2(\beta\mu B) + e^{-4\beta\varepsilon}\right]^{1/2}}$$

$$M(T,J,H) = \frac{N\mu \sinh(\beta\mu B)}{\left[\sinh^2(\beta\mu B) + e^{-4\beta\varepsilon}\right]^{1/2}}$$



Mean field approximation for 1-dimensional Ising model

Exact Hamiltonian:

$$\hat{H}_{Ising} = -\varepsilon \sum_{i=1}^{N} s_i s_{i+1} - \mu B \sum_{i=1}^{N} s_i$$

Mean field approximation:

$$\hat{H}^{MF}_{\text{Ising}} = -\varepsilon \sum_{i=1}^{N} s_i \langle s_i \rangle - \mu B \sum_{i=1}^{N} s_i$$

$$= -\left(\varepsilon \langle s_i \rangle + \mu B\right) \sum_{i=1}^{N} s_i$$

$$\equiv -H_{eff} \sum_{i=1}^{N} s_i$$

Mean field partition function and Free energy:

$$A = -kT \ln\left(Z_1\right)^N = -NkT \ln Z_1 = -NkT \ln\left(2\cosh(\beta H_{eff})\right)$$

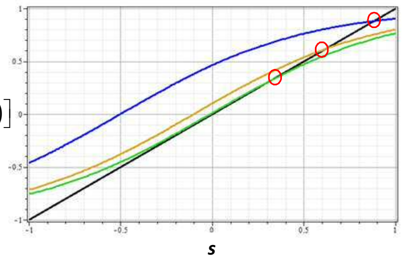
$$H_{eff} = \varepsilon \langle s_i \rangle + \mu B$$

Consistency condition:

$$\langle s_i \rangle = \frac{1}{Z_1} \sum_{s_i} s_i e^{-\beta H_{eff} s_i} = \tanh\left[\beta\left(\varepsilon \langle s_i \rangle + \mu B\right)\right]$$

Consistency condition:

$$\langle s_i \rangle = \tanh\left[\beta\left(\varepsilon\langle s_i\rangle + \mu B\right)\right]$$



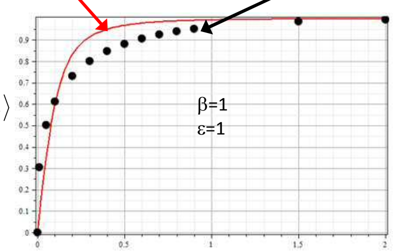
One dimensional Ising model with periodic boundary conditions:

Exact solution:

$$\langle s_i \rangle \equiv \frac{M}{N} = \frac{\sinh(\beta\mu B)}{\left[\sinh^2(\beta\mu B) + e^{-4\beta\varepsilon}\right]^{1/2}}$$

Mean field solution:

$$\langle s_i \rangle = \tanh\left[\beta\left(\varepsilon\langle s_i\rangle + \mu B\right)\right]$$



Extension of mean field analysis to more complicated geometries

Ising model:

$$\hat{H}_{Ising} = \sum_{i,j(nn)}^{N} \epsilon_{ij} s_i s_j - \mu B \sum_{i=1}^{N} s_i \Rightarrow -\epsilon \sum_{i,j(nn)}^{N} s_i s_j - \mu B \sum_{i=1}^{N} s_i$$

Ising model in mean field approximation:

$$\hat{H}_{Ising}^{MF} = -\epsilon \frac{\nu}{2} \sum_{i}^{N} s_i \langle s_j \rangle - \mu B \sum_{i=1}^{N} s_i$$

$\nu \equiv$ number of nearest neighbors

$$\hat{H}_{Ising}^{MF} = -\left(\epsilon \frac{\nu}{2} \langle s_j \rangle + \mu B\right) \sum_{i=1}^{N} s_i \equiv -H_{eff} \sum_{i=1}^{N} s_i$$

Extension of mean field analysis to more complicated geometries -- continued

Mean field partition function and Free energy:

$$A = -kT \ln\left(Z_1\right)^N = -NkT \ln Z_1 = -NkT \ln\left(2\cosh(\beta H_{eff})\right)$$

$$H_{eff} = \varepsilon \frac{\nu}{2}\langle s_i \rangle + \mu B$$

Consistency condition:

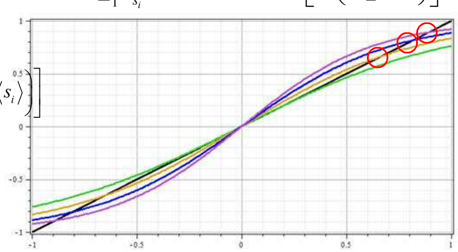
$$\langle s_i \rangle = \frac{1}{Z_1}\sum_{s_i} s_i e^{-\beta H_{eff} s_i} = \tanh\left[\beta\left(\varepsilon \frac{\nu}{2}\langle s_i \rangle + \mu B\right)\right]$$

Extension of mean field analysis to more complicated geometries -- continued

Consistency condition for B=0:

$$\langle s_i \rangle = \frac{1}{Z_1}\sum_{s_i} s_i e^{-\beta H_{eff} s_i} = \tanh\left[\beta\left(\varepsilon \frac{\nu}{2}\langle s_i \rangle\right)\right]$$

$$\tanh\left[\beta\left(\varepsilon \frac{\nu}{2}\langle s_i \rangle\right)\right]$$



Extension of mean field analysis to more complicated geometries -- continued

Consistency condition for B=0:

Define: $s_0 = \tanh\left[\beta\left(\varepsilon \frac{\nu}{2} s_0\right)\right]$

$$Z_N = \begin{cases} (2)^N & \text{for } \langle s \rangle = 0 \\ \left(2\cosh(\beta\varepsilon\nu/2)\right)^N & \text{for } \langle s \rangle = \pm s_0 \end{cases}$$

$$U = -\left(\frac{\partial \ln(Z_N)}{\partial \beta}\right) = -\frac{1}{2} N\nu\varepsilon s_0^2$$

Extension of mean field analysis to more complicated geometries -- continued

Consistency condition for B=0:

Define: $s_0 = \tanh\left[\beta\left(\varepsilon \frac{\nu}{2} s_0\right)\right]$

Heat capacity:

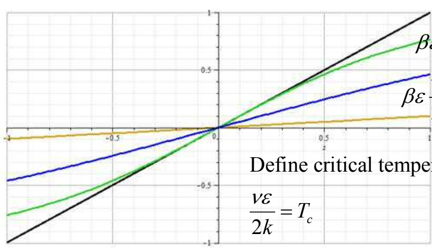
$$C_N = \left(\frac{\partial U}{\partial T}\right)_N = -\left(\frac{\partial \ln(Z_N)}{\partial \beta}\right) = N\nu\varepsilon\beta^2 s_0 \left(\frac{\partial s_0}{\partial \beta}\right)_N$$

$$C_N = \frac{Nk\nu^2\varepsilon^2\beta^2 s_0^2}{2\cosh^2(\beta\nu\varepsilon s_0/2) - \beta\nu\varepsilon}$$

Extension of mean field analysis to more complicated geometries -- continued

For: $s_0 = \tanh\left[\beta\left(\varepsilon \frac{\nu}{2} s_0\right)\right]$

Note that there is no solution for $\beta\varepsilon \frac{\nu}{2} < 1$:



Define critical temperature

$$\frac{\nu\varepsilon}{2k} = T_c$$

Extension of mean field analysis to more complicated geometries -- continued

$$T_c \equiv \frac{\nu\varepsilon}{2k}$$

Heat capacity in terms of critical temperature:

$$C_N = \begin{cases} \dfrac{2Nks_0^2\left(T_c/T\right)^2}{\cosh^2\left(s_0\left(T_c/T\right)\right) - T_c/T} & \text{for } T < T_c \\ 0 & \text{for } T > T_c \end{cases}$$